



Full wwPDB X-ray Structure Validation Report i

Nov 19, 2023 – 07:46 PM JST

PDB ID : 6M4R
Title : Structure of Human Serum Albumin
Authors : Xiang, W.; Su, J.
Deposited on : 2020-03-09
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

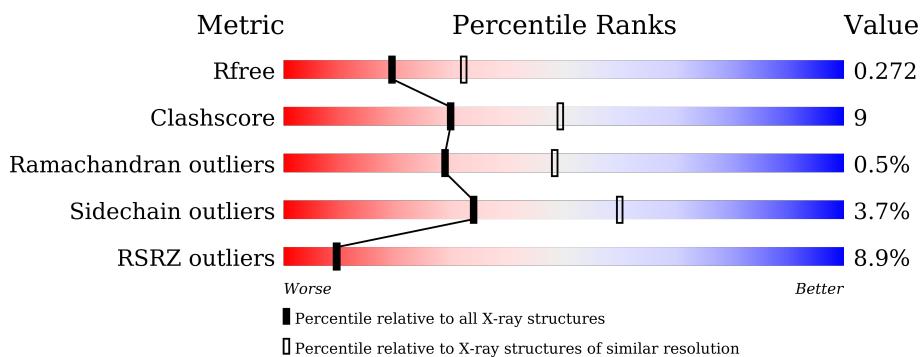
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

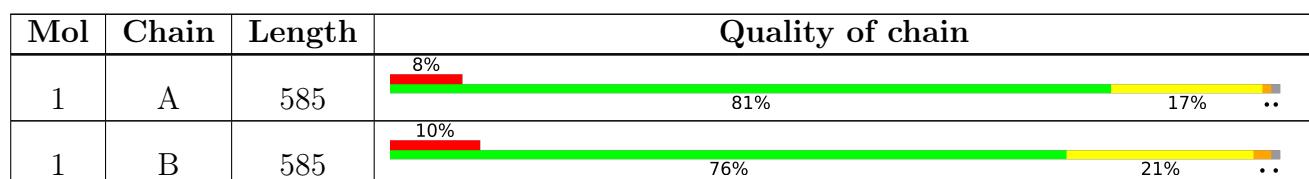
The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4567	2883	771	872	41			

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf				
1	B	579	Total	C	N	O	S	0	0	0
			4544	2866	767	870	41			

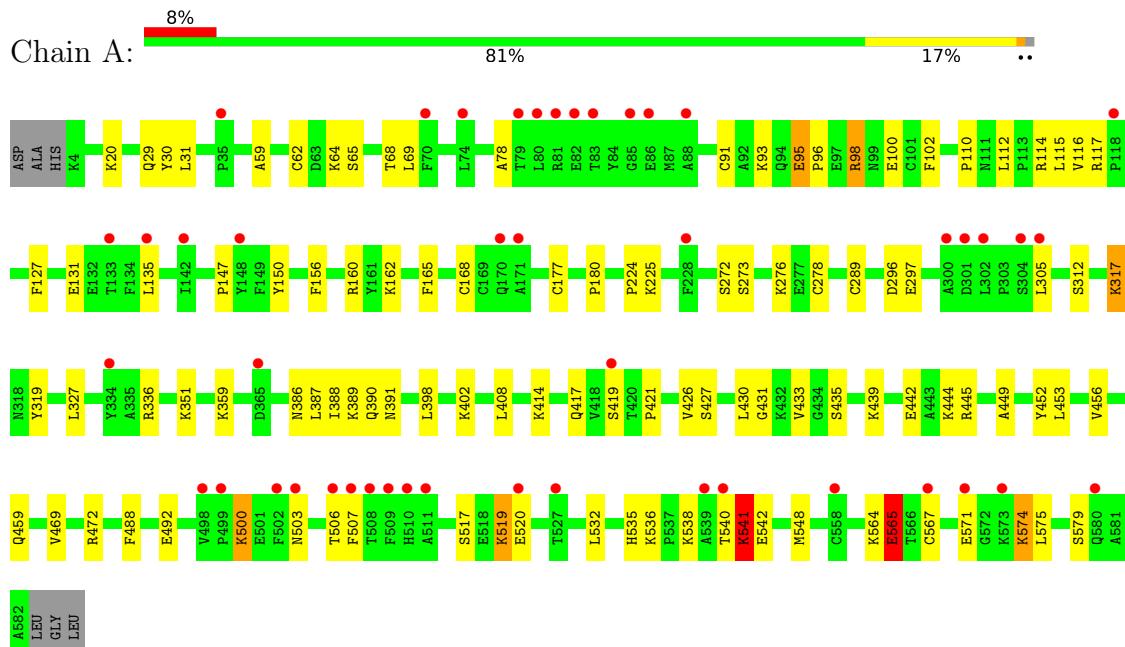
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	37	Total	O	0	0
			37	37		

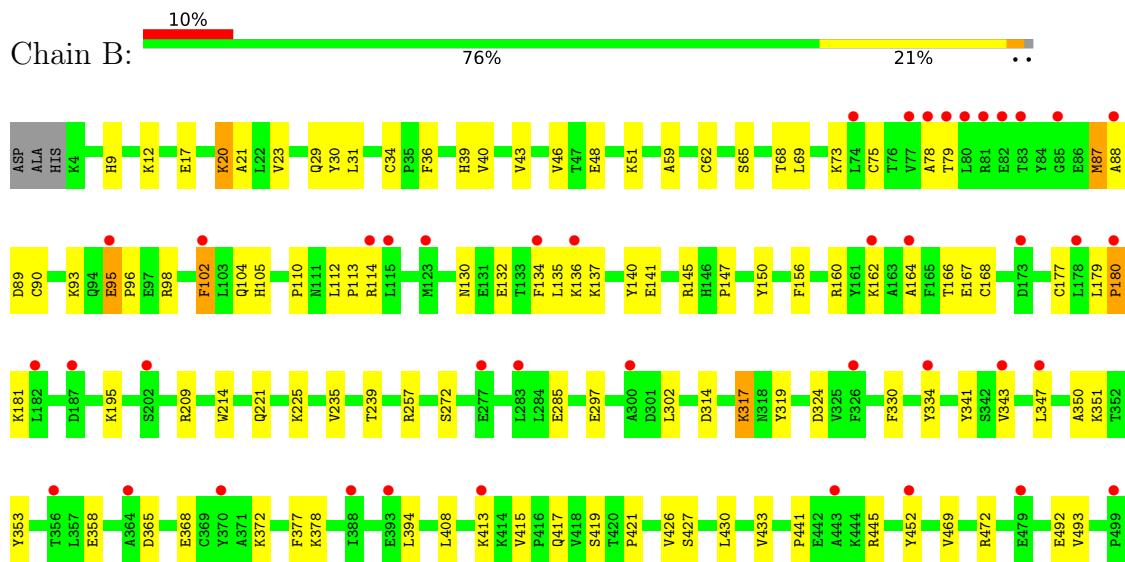
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serum albumin



- Molecule 1: Serum albumin





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.66 Å 59.10 Å 86.81 Å 90.10° 90.04° 103.60°	Depositor
Resolution (Å)	19.76 – 2.49 19.76 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.1 (19.76-2.49) 97.6 (19.76-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.62 (at 2.50 Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R , R_{free}	0.232 , 0.274 0.232 , 0.272	Depositor DCC
R_{free} test set	2021 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9182	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.28	0/4655	0.44	0/6285
1	B	0.31	0/4631	0.45	0/6256
All	All	0.29	0/9286	0.44	0/12541

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4567	0	4462	76	0
1	B	4544	0	4415	92	0
2	A	34	0	0	3	0
2	B	37	0	0	4	0
All	All	9182	0	8877	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:CB	1:A:96:PRO:HD3	1.48	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:HB3	1:B:96:PRO:CD	1.38	1.36
1:A:95:GLU:CB	1:A:96:PRO:CD	2.16	1.23
1:B:95:GLU:CB	1:B:96:PRO:CD	2.19	1.20
1:B:95:GLU:CB	1:B:96:PRO:HD3	1.71	1.19
1:B:134:PHE:HA	1:B:137:LYS:HD3	1.55	0.87
1:A:442:GLU:HA	1:A:445:ARG:HB2	1.61	0.82
1:A:519:LYS:NZ	1:A:520:GLU:HG2	1.95	0.82
1:B:540:THR:HG23	1:B:543:GLN:NE2	1.96	0.81
1:A:433:VAL:HG12	1:A:452:TYR:HD2	1.46	0.80
1:B:95:GLU:HB3	1:B:96:PRO:HD3	0.77	0.76
1:B:541:LYS:HD2	1:B:541:LYS:H	1.51	0.76
1:B:114:ARG:HH11	1:B:114:ARG:HG3	1.52	0.74
1:A:115:LEU:HD22	1:A:117:ARG:HD3	1.70	0.73
1:A:317:LYS:HD2	1:A:317:LYS:H	1.51	0.72
1:A:575:LEU:HD23	1:A:575:LEU:O	1.88	0.72
1:B:95:GLU:CB	1:B:96:PRO:HD2	2.17	0.72
1:A:115:LEU:CD2	1:A:117:ARG:HD3	2.23	0.69
1:B:472:ARG:NH2	1:B:492:GLU:O	2.24	0.69
1:B:541:LYS:HD2	1:B:541:LYS:N	2.08	0.68
1:B:433:VAL:HG12	1:B:452:TYR:HD2	1.58	0.68
1:B:540:THR:HG22	1:B:543:GLN:HG3	1.77	0.66
1:A:115:LEU:CD2	1:A:117:ARG:HG3	2.27	0.65
1:A:519:LYS:HZ2	1:A:520:GLU:HG2	1.60	0.64
1:A:575:LEU:HD23	1:A:575:LEU:C	2.17	0.64
1:B:551:PHE:CE1	1:B:575:LEU:HD11	2.33	0.64
1:A:500:LYS:O	1:A:535:HIS:ND1	2.31	0.63
1:B:112:LEU:HD12	1:B:145:ARG:HG3	1.80	0.63
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.81	0.63
1:A:386:ASN:O	1:A:390:GLN:HG3	1.98	0.62
1:A:115:LEU:HD22	1:A:117:ARG:CD	2.29	0.62
1:B:544:LEU:HG	2:B:616:HOH:O	1.98	0.62
1:B:110:PRO:HB2	1:B:112:LEU:HG	1.82	0.62
1:B:79:THR:HG23	1:B:88:ALA:HB1	1.83	0.61
1:A:387:LEU:O	1:A:391:ASN:ND2	2.25	0.61
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.82	0.61
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.01	0.60
1:A:503:ASN:OD1	1:A:506:THR:N	2.35	0.60
1:A:433:VAL:HG12	1:A:452:TYR:CD2	2.33	0.60
1:B:48:GLU:OE2	1:B:51:LYS:NZ	2.33	0.60
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.42	0.60
1:B:417:GLN:HB3	1:B:469:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:CE2	1:A:165:PHE:HB3	2.37	0.60
1:A:319:TYR:HE1	1:A:327:LEU:HD11	1.67	0.59
1:B:29:GLN:HG2	1:B:147:PRO:HA	1.84	0.59
1:B:20:LYS:HD2	1:B:21:ALA:N	2.17	0.59
1:B:114:ARG:HG3	1:B:114:ARG:NH1	2.17	0.59
1:A:30:TYR:CD1	1:A:102:PHE:HB3	2.38	0.58
1:A:135:LEU:HD11	1:A:162:LYS:HB3	1.86	0.58
1:B:87:MET:HB3	1:B:105:HIS:CD2	2.38	0.58
1:A:472:ARG:NH2	1:A:492:GLU:O	2.37	0.57
1:A:114:ARG:HG2	1:A:116:VAL:HG23	1.87	0.57
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.87	0.57
1:A:430:LEU:O	1:A:433:VAL:HG22	2.05	0.56
1:B:413:LYS:HB3	1:B:493:VAL:HG22	1.88	0.56
1:B:319:TYR:OH	1:B:358:GLU:OE1	2.23	0.56
1:B:314:ASP:HA	1:B:317:LYS:HG3	1.87	0.56
1:B:209:ARG:HH22	1:B:324:ASP:CG	2.09	0.55
1:B:225:LYS:HE2	1:B:297:GLU:O	2.07	0.55
1:B:433:VAL:HG12	1:B:452:TYR:CD2	2.39	0.55
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.47	0.54
1:B:36:PHE:O	1:B:40:VAL:HG23	2.07	0.54
1:B:168:CYS:CB	1:B:177:CYS:SG	2.95	0.54
1:B:162:LYS:O	1:B:166:THR:HG23	2.07	0.54
1:A:414:LYS:NZ	1:A:488:PHE:O	2.30	0.54
1:A:575:LEU:HD23	1:A:579:SER:OG	2.07	0.54
1:B:17:GLU:HG3	1:B:20:LYS:HE3	1.90	0.53
1:B:75:CYS:HA	1:B:78:ALA:HB3	1.91	0.53
1:A:114:ARG:HH22	1:A:519:LYS:HZ1	1.56	0.53
1:B:540:THR:HA	1:B:543:GLN:CD	2.28	0.53
1:A:390:GLN:NE2	2:A:611:HOH:O	2.41	0.52
1:B:365:ASP:CG	1:B:368:GLU:HG3	2.29	0.52
1:A:64:LYS:HB2	1:A:69:LEU:HD21	1.92	0.52
1:A:442:GLU:HG3	1:A:445:ARG:HH21	1.73	0.52
1:B:87:MET:HB3	1:B:105:HIS:CG	2.45	0.52
1:B:73:LYS:NZ	2:B:606:HOH:O	2.33	0.52
1:B:104:GLN:NE2	2:B:608:HOH:O	2.36	0.52
1:A:68:THR:HA	1:A:98:ARG:NH2	2.26	0.51
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.93	0.51
1:B:168:CYS:CB	1:B:177:CYS:HG	2.17	0.51
1:B:132:GLU:O	1:B:136:LYS:HG3	2.11	0.51
1:B:427:SER:HA	1:B:430:LEU:HD12	1.92	0.51
1:A:417:GLN:HB3	1:A:469:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:N	1:B:180:PRO:HD2	2.26	0.51
1:B:23:VAL:HG11	1:B:46:VAL:HG21	1.92	0.50
1:B:573:LYS:O	1:B:576:VAL:HG12	2.12	0.50
1:A:433:VAL:HG21	1:A:453:LEU:HD21	1.93	0.50
1:A:224:PRO:O	1:A:336:ARG:NH2	2.41	0.49
1:B:430:LEU:O	1:B:433:VAL:HG22	2.12	0.49
1:B:528:ALA:HB1	1:B:551:PHE:HE2	1.77	0.49
1:B:65:SER:O	1:B:69:LEU:HG	2.13	0.49
1:B:95:GLU:HB2	1:B:96:PRO:HD2	1.95	0.49
1:B:408:LEU:HD13	1:B:427:SER:HB2	1.94	0.48
1:A:30:TYR:CE1	1:A:102:PHE:HB3	2.48	0.48
1:A:536:LYS:HG2	1:A:538:LYS:O	2.13	0.48
1:A:574:LYS:HA	1:A:574:LYS:HD3	1.54	0.48
1:A:419:SER:OG	1:A:421:PRO:HD2	2.13	0.48
1:B:347:LEU:O	1:B:351:LYS:HG2	2.14	0.48
1:A:435:SER:N	2:A:601:HOH:O	2.36	0.47
1:B:541:LYS:HD2	1:B:543:GLN:HG2	1.97	0.47
1:B:419:SER:OG	1:B:421:PRO:HD2	2.15	0.47
1:B:181:LYS:H	1:B:181:LYS:HG2	1.33	0.46
1:A:319:TYR:CE1	1:A:327:LEU:HD11	2.50	0.46
1:A:439:LYS:HE3	1:A:439:LYS:HA	1.97	0.46
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.98	0.46
1:B:87:MET:C	1:B:89:ASP:N	2.69	0.46
1:A:114:ARG:HH22	1:A:519:LYS:NZ	2.12	0.45
1:B:221:GLN:NE2	1:B:341:TYR:O	2.49	0.45
1:A:131:GLU:O	1:A:135:LEU:HD23	2.15	0.45
1:B:9:HIS:HA	1:B:12:LYS:HE2	1.97	0.45
1:B:195:LYS:HD2	1:B:195:LYS:HA	1.81	0.45
1:A:564:LYS:O	1:A:565:GLU:HG3	2.17	0.45
1:B:557:LYS:NZ	1:B:567:CYS:SG	2.89	0.45
1:A:65:SER:O	1:A:69:LEU:HG	2.17	0.45
1:A:567:CYS:O	1:A:571:GLU:HB2	2.17	0.45
1:B:394:LEU:O	2:B:601:HOH:O	2.21	0.45
1:B:39:HIS:O	1:B:43:VAL:HG23	2.16	0.44
1:B:90:CYS:HA	1:B:93:LYS:HG2	1.98	0.44
1:B:415:VAL:HG23	1:B:415:VAL:O	2.16	0.44
1:B:542:GLU:HG3	1:B:545:LYS:CB	2.47	0.44
1:A:431:GLY:O	2:A:601:HOH:O	2.21	0.44
1:B:141:GLU:O	1:B:145:ARG:HD2	2.18	0.44
1:B:503:ASN:O	1:B:506:THR:HG22	2.17	0.44
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LEU:C	1:A:575:LEU:CD2	2.85	0.44
1:A:168:CYS:HB3	1:A:177:CYS:HB3	1.87	0.44
1:B:31:LEU:HD11	1:B:78:ALA:HB2	2.00	0.44
1:A:426:VAL:HG13	1:A:456:VAL:HG12	1.99	0.44
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.86	0.43
1:A:388:ILE:HD13	1:A:449:ALA:HB3	2.00	0.43
1:A:351:LYS:HA	1:A:351:LYS:HD2	1.86	0.43
1:B:87:MET:C	1:B:89:ASP:H	2.21	0.43
1:B:525:LYS:HE3	1:B:548:MET:HG3	1.99	0.43
1:A:575:LEU:HD23	1:A:579:SER:HG	1.83	0.43
1:B:517:SER:OG	1:B:518:GLU:N	2.51	0.43
1:A:541:LYS:HB2	1:A:542:GLU:H	1.71	0.43
1:A:386:ASN:HA	1:A:389:LYS:HG2	2.00	0.43
1:B:164:ALA:HB1	1:B:181:LYS:HD3	2.00	0.43
1:B:156:PHE:CE2	1:B:160:ARG:HD2	2.54	0.42
1:A:398:LEU:O	1:A:402:LYS:HD2	2.20	0.42
1:B:113:PRO:O	1:B:145:ARG:NH1	2.50	0.42
1:A:156:PHE:CE2	1:A:160:ARG:HD2	2.54	0.42
1:A:519:LYS:HZ1	1:A:520:GLU:HG2	1.81	0.42
1:A:439:LYS:HD2	1:A:439:LYS:N	2.34	0.42
1:B:30:TYR:CD1	1:B:102:PHE:HB3	2.55	0.42
1:B:353:TYR:HB2	1:B:377:PHE:HZ	1.84	0.42
1:A:225:LYS:HE3	1:A:297:GLU:O	2.19	0.42
1:B:330:PHE:HE2	1:B:350:ALA:HA	1.85	0.42
1:A:532:LEU:HD21	1:A:548:MET:CE	2.50	0.42
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.35	0.42
1:B:134:PHE:O	1:B:137:LYS:HB2	2.19	0.42
1:B:378:LYS:HB3	1:B:378:LYS:HE3	1.58	0.41
1:A:115:LEU:CD2	1:A:117:ARG:CG	2.97	0.41
1:B:135:LEU:HD11	1:B:162:LYS:HB3	2.01	0.41
1:A:78:ALA:HB3	1:A:91:CYS:SG	2.60	0.41
1:B:235:VAL:O	1:B:239:THR:OG1	2.25	0.41
1:A:536:LYS:HG2	1:A:540:THR:HG23	2.01	0.41
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.54	0.41
1:B:426:VAL:O	1:B:430:LEU:HG	2.21	0.41
1:B:441:PRO:O	1:B:445:ARG:HB2	2.21	0.41
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.03	0.41
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.56	0.41
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.86	0.41
1:A:156:PHE:CZ	1:A:160:ARG:HD2	2.56	0.41
1:B:68:THR:HA	1:B:98:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLU:HG3	1:B:545:LYS:HB2	2.03	0.40
1:B:167:GLU:OE1	1:B:181:LYS:NZ	2.54	0.40
1:B:168:CYS:HG	1:B:177:CYS:CB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	577/585 (99%)	547 (95%)	26 (4%)	4 (1%)	22 39
1	B	577/585 (99%)	549 (95%)	26 (4%)	2 (0%)	41 61
All	All	1154/1170 (99%)	1096 (95%)	52 (4%)	6 (0%)	29 48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	541	LYS
1	B	95	GLU
1	A	565	GLU
1	B	180	PRO
1	A	180	PRO

5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/511 (98%)	479 (96%)	19 (4%)	33 58
1	B	492/511 (96%)	474 (96%)	18 (4%)	34 60
All	All	990/1022 (97%)	953 (96%)	37 (4%)	34 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	93	LYS
1	A	98	ARG
1	A	150	TYR
1	A	272	SER
1	A	273	SER
1	A	276	LYS
1	A	312	SER
1	A	317	LYS
1	A	359	LYS
1	A	444	LYS
1	A	459	GLN
1	A	500	LYS
1	A	507	PHE
1	A	517	SER
1	A	519	LYS
1	A	541	LYS
1	A	565	GLU
1	A	574	LYS
1	B	20	LYS
1	B	87	MET
1	B	102	PHE
1	B	130	ASN
1	B	140	TYR
1	B	150	TYR
1	B	257	ARG
1	B	272	SER
1	B	317	LYS
1	B	334	TYR
1	B	372	LYS
1	B	505	GLU
1	B	507	PHE
1	B	517	SER
1	B	538	LYS
1	B	540	THR

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Mol	Chain	Res	Type
1	B	541	LYS
1	B	554	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	B	268	GLN
1	B	367	HIS
1	B	503	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	579/585 (98%)	0.70	46 (7%) 12 12	36, 62, 95, 135	0
1	B	579/585 (98%)	0.74	57 (9%) 7 7	36, 63, 92, 132	0
All	All	1158/1170 (98%)	0.72	103 (8%) 9 9	36, 63, 94, 135	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	ALA	18.6
1	A	539	ALA	15.1
1	B	81	ARG	14.2
1	B	80	LEU	8.6
1	B	83	THR	8.5
1	B	77	VAL	8.2
1	A	83	THR	7.6
1	A	508	THR	6.9
1	B	502	PHE	6.7
1	B	85	GLY	6.5
1	A	300	ALA	5.8
1	A	81	ARG	5.3
1	B	114	ARG	5.2
1	A	302	LEU	5.2
1	B	79	THR	5.1
1	B	576	VAL	4.8
1	B	115	LEU	4.7
1	B	134	PHE	4.6
1	B	82	GLU	4.6
1	B	283	LEU	4.4
1	B	187	ASP	4.3
1	B	364	ALA	4.2
1	A	509	PHE	4.1
1	B	544	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	510	HIS	3.9
1	A	567	CYS	3.8
1	B	509	PHE	3.7
1	A	79	THR	3.7
1	A	85	GLY	3.7
1	A	304	SER	3.7
1	B	564	LYS	3.6
1	A	511	ALA	3.6
1	B	277	GLU	3.3
1	B	443	ALA	3.3
1	A	82	GLU	3.3
1	A	580	GLN	3.2
1	A	133	THR	3.2
1	B	178	LEU	3.1
1	B	173	ASP	3.1
1	B	343	VAL	3.1
1	A	170	GLN	3.1
1	B	553	ALA	3.1
1	B	356	THR	3.0
1	A	573	LYS	3.0
1	A	228	PHE	3.0
1	A	171	ALA	3.0
1	B	300	ALA	3.0
1	B	347	LEU	3.0
1	A	507	PHE	2.9
1	A	558	CYS	2.9
1	B	393	GLU	2.8
1	B	499	PRO	2.8
1	B	74	LEU	2.8
1	A	301	ASP	2.8
1	A	86	GLU	2.7
1	B	551	PHE	2.7
1	B	88	ALA	2.7
1	A	118	PRO	2.6
1	A	520	GLU	2.6
1	B	180	PRO	2.6
1	B	413	LYS	2.6
1	B	182	LEU	2.6
1	A	419	SER	2.5
1	B	370	TYR	2.5
1	B	162	LYS	2.5
1	A	365	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	506	THR	2.5
1	B	164	ALA	2.5
1	A	334	TYR	2.4
1	A	135	LEU	2.4
1	A	503	ASN	2.4
1	A	142	ILE	2.4
1	B	136	LYS	2.4
1	B	538	LYS	2.4
1	A	74	LEU	2.4
1	B	500	LYS	2.3
1	A	35	PRO	2.3
1	B	123	MET	2.3
1	B	326	PHE	2.3
1	B	508	THR	2.3
1	B	102	PHE	2.3
1	B	334	TYR	2.3
1	A	88	ALA	2.3
1	B	535	HIS	2.3
1	B	202	SER	2.3
1	A	571	GLU	2.3
1	B	567	CYS	2.2
1	B	95	GLU	2.2
1	B	532	LEU	2.2
1	B	452	TYR	2.1
1	A	499	PRO	2.1
1	A	148	TYR	2.1
1	A	80	LEU	2.1
1	B	78	ALA	2.1
1	B	546	ALA	2.1
1	A	540	THR	2.1
1	A	502	PHE	2.1
1	B	479	GLU	2.1
1	A	527	THR	2.0
1	B	388	ILE	2.0
1	A	305	LEU	2.0
1	A	498	VAL	2.0
1	A	70	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.